Energy Estimates for Low Regularity Bilinear Schrödinger Equations ⋆

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Abstract: This paper presents an energy estimate in terms of the total variation of the control for bilinear infinite dimensional quantum systems with unbounded potentials. These estimates allow a rigorous construction of propagators associated with controls of bounded variation. Moreover, upper bounds of the error made when replacing the infinite dimensional system by its finite dimensional Galerkin approximations is presented.

Keywords: Bilinear systems, quantum systems, well-posedness, approximation.

1. INTRODUCTION

1.1 Physical context

The state of a quantum system evolving in a Riemannian manifold Ω is described by its *wave function*, a point ψ in $L^2(\Omega, \mathbf{C})$. When the system is submitted to an electric field (e.g., a laser), the time evolution of the wave function is given, under the dipolar approximation and neglecting decoherence, by the Schrödinger bilinear equation:

$$\mathrm{i}\frac{\partial \psi}{\partial t} = (-\Delta + V(x))\psi(x,t) + u(t)W(x)\psi(x,t) \qquad (1)$$

where Δ is the Laplace-Beltrami operator on Ω, V and W are real potential accounting for the properties of the free system and the control field respectively, while the real function of the time u accounts for the intensity of the laser.

In view of applications (for instance in NMR), it is important to know whether and how it is possible to chose a suitable control $u : [0,T] \to \mathbf{R}$ in order to steer (1) from a given initial state to a given target. This question has raised considerable interest in the community in the last decade. After the negative results of Ball et al. (1982) and Turinici (2000) excluding exact controllability on the natural domain of the operator $-\Delta + V$ when W is bounded, the first, and at this day the only one, description of the attainable set for an example of bilinear quantum system was obtained by (Beauchard (2005); Beauchard and Coron (2006)). Further investigations of the approximate controllability of (1) were conducted using Lyapunov techniques (Nersesyan (2010, 2009); Beauchard and Nersesyan (2010); Beauchard et al. (2007); Mirrahimi et al. (2005); Mirrahimi (2006)) and geometric techniques (Chambrion et al. (2009); Boscain et al. (2012)).

In most of the references cited above, the potentials V and W in (1) are bounded. The very general (and irregular) systems considered by Boscain et al. (2012) allow to define the solutions of (1) for piecewise constant controls only. The aim of this paper is to present a coherent framework to deal with unbounded potentials in (1). This includes a rigorous definition of the solution of (1) for control that are not necessarily piecewise constant and the extension of some quantitative energy estimates.

1.2 Abstract framework and notations

We reformulate the control problem in more abstract framework, in such a way that we can use some of the powerful tools of functional analysis. In a separable Hilbert space H, we consider a pair (A, B) of (possibly unbounded) linear operators that satisfy Hypothesis 1

Hypothesis 1. (A, B) is a pair of linear operators such that

(1) A is skew-adjoint on its domain $D(A)$;
(2) $\mathrm{i}A$ is bounded from below;
(3) B is skew-symmetric;
(4) there exists $a, b \geq 0$ such that $\|B\psi\| \leq a\|A\psi\| + b\|\psi\|$ for any ψ in $D(A)$.

Following Kato (1953), Hypothesis 1 is the minimal framework for our developments. For many examples encoun-

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tered in the physics literature, A has a discrete spectrum and we will consider the more restrictive Hypothesis 2.

Hypothesis 2. $(A, B, (\phi_j)_{j\in\mathbf{N}}, \alpha)$ is a quadruple such that

(1) (A, B) satisfies Hypothesis 1;
(2) $(\phi_j)_{j\in\mathbf{N}}$ is a Hilbert basis of H;
(3) $0 \leq \alpha \leq 1$;
(4) A has discrete spectrum $(-\mathrm{i}\lambda_j)_{j\in\mathbf{N}}$ with $\lambda_j \to +\infty$ as $j \to \infty$;
(5) for any j in $\mathbf{N}$, $A\phi_j = -\mathrm{i}\lambda_j\phi_j$;
(6) there exists $d \geq 0$ such that $\|B\psi\| \leq d\||A|^\alpha\psi\|$ for any ψ in $D(|A|^\alpha)$.

Thanks to the Kato-Rellich theorem (see Kato (1995)), Hypotheses 1.1, 1.3 and 1.4 imply that, for any u in $(-1/a, 1/a)$, $A + uB$ is skew-adjoint with domain $D(A)$ and generates a unitary propagator $t \mapsto e^{t(A+uB)}$. In particular, this allows to define by concatenation the propagator $\Upsilon^u : t \mapsto \Upsilon^u_t$ for the control system

$$\frac{\mathrm{d}\psi}{\mathrm{d}t} = (A + u(t)B)\psi \tag{2}$$

for u piecewise constant u taking value in $(-1/a, 1/a)$.

Recall that a function $u : [0, T] \to \mathbf{R}$ has *bounded variation* (or is BV) if there exists a constant C such that, for any partition $0 = a_0 < a_1 < \ldots < a_n = T$ of $[0, T]$, $\sum_{k=1}^n |u(a_k) - u(a_{k-1})| < C$. The smallest C satisfying this property for any partition of $[0, T]$ is the *total variation* of u, denoted $TV_{[0,T]}(u)$.

We define the set $\mathcal{U}$ of the functions $u : \mathbf{R} \to \mathbf{R}$ with bounded variation such that $u(t) = 0$ for $t \leq 0$. In $\mathcal{U}$, the sequence $(u_n)_{n\in\mathbf{N}}$ converges to u if $\sup_n TV_{\mathbf{R}}(u_n) \leq TV_{\mathbf{R}}(u)$ and $u_n(t)$ tends to $u(t)$ as n goes to infinity for almost any t in $\mathbf{R}$.

1.3 Contribution of this paper

This paper presents a rigorous yet elementary construction of the solutions of (2) associated with controls of bounded variation, inspired from Kato (1953). Among other byproducts of our energy estimates, we give a lower bound for the number of switches needed to steer (2) from a given source to a given target using controls with value in $\{0, 1\}$ and we give an upper bound of the error made when one replaces the original infinite dimensional system (2) by one of its finite dimensional Galerkin approximation. Such estimates are instrumental in practice, both for theoretical analysis, design of control laws and numerical simulations.

The strength of our results is the relative generality of our assumptions. In this sense, this paper may be seen as an extension of the results of Boussaïd et al. (2012b) to systems that are not *weakly-coupled* (according to (Boussaïd et al., 2013, Definition 1)).

1.4 Content of the paper

The first part of the paper (Section 2) is concerned with the construction of the solutions of (2) for controls with bounded variation. The key point of this construction is an energy estimate in terms of the total variation of the control (see Proposition 3). The second part of the paper (Section 3) presents some consequences of this energy estimate in terms of approximation of the original infinite dimensional system by its finite dimensional dynamics. Finally, we apply our results to various types of quantum oscillators encountered in the physics literature (Section 4).

2. CONSTRUCTION OF THE PROPAGATORS

To begin with, we consider the simple case where $\|B\psi\| \leq a\|A\psi\|$ for any ψ in $D(A)$. The general case of operators B relatively bounded with respect to A satisfying Hypothesis 1.4 will be treated in Subsection 2.3.

2.1 Estimates on the A norm

For any ψ in $D(A)$, for any u in $\mathbf{R}$ such that $a|u| < 1$,

$$\|B\psi\| \leq a\|A\psi\| \tag{3}$$
$$\leq a(\|(A + uB)\psi\| + |u|\|B\psi\|) \tag{4}$$

Hence,

$$(1 - a|u|)\|B\psi\| \leq a\|(A + uB)\psi\| \tag{5}$$
$$\|B\psi\| \leq \frac{a}{1 - |u|a}\|(A + uB)\psi\| \tag{6}$$

For any u_1, u_2 in $(-1/a, 1/a)$, t in $\mathbf{R}$ and ψ in $D(A)$, ψ is in $D(A + u_2B)$ by Hypothesis 1.4. Hence, $e^{t(A+u_2B)}\psi$ belongs to $D(A+u_2B) = D(A) = D(A+u_1B)$. Moreover,

$$\begin{aligned}
&\|(A + u_1B)e^{t(A+u_2B)}\psi\| \\
&\leq \|(A + u_2B)e^{t(A+u_2B)}\psi\| + \|(u_1 - u_2)Be^{t(A+u_2B)}\psi\| \\
&\leq \|e^{t(A+u_2B)}(A + u_2B)\psi\| \\
&\qquad + |u_1 - u_2|\frac{a}{1 - |u_2|a}\|(A + u_2B)e^{t(A+u_2B)}\psi\|
\end{aligned}$$

and hence

$$\begin{aligned}
&\|(A + u_1B)e^{t(A+u_2B)}\psi\| \\
&\leq \left(1 + \frac{|u_1 - u_2|\|B\|_A}{1 - |u_1|a}\right)\|(A + u_2B)\psi\|
\end{aligned}$$

and

$$\|(A + u_1B)\psi\| \leq \left(1 + \frac{|u_1 - u_2|a}{1 - |u_1|a}\right)\|(A + u_2B)\psi\|$$

Let $u^* > 0$ be given such that $|u^*| < 1/a$. For any $t \geq 0$, for any u_1, u_2 in $(-u^*, u^*)$ one has, with $\Gamma = \frac{a}{1-|u^*|a}$,

$$\begin{aligned}
&\|(A + u_1B)e^{t(A+u_2B)}\psi\| \\
&\qquad \leq \exp\left(\Gamma|u_2 - u_1|\right)\|(A + u_2B)\psi\|.
\end{aligned}$$

Consider now a piecewise constant control $u : [0, T] \to (-1/a, 1/a)$ taking value u_j for time t_j, $t_j \geq 0$ $1 \leq j \leq p$, $p \in \mathbf{N}$. We get by concatenation, for any ψ in $D(A)$,

$$
\begin{aligned}
&\|A\Upsilon^u_{T,0}\psi\| \\
&\leq \exp(\Gamma|u_p|) \times \\
&\quad \times\|(A+u_pB)e^{t_p(A+u_pB)}e^{t_{p-1}(A+u_{p-1}B)}\cdots e^{t_1(A+u_1B)}\psi\| \\
&\leq \exp(\Gamma|u_p|)\left[\prod_{j=1}^{p}\exp\left(\Gamma|u_j-u_{j+1}|\right)\right]\exp(\Gamma|u_1|)\|A\psi\| \\
&\leq \exp(2\Gamma TV_{[0,T]}(u))\|A\psi\|.
\end{aligned}
$$

We obtain, similarly to Kato (1953), the following result.

Proposition 3. For any $\delta \in (0,1)$, let (A,B) satisfy Hypothesis 1. Then, for any piecewise constant $u : [0,T] \to (-(1-\delta)/a, (1-\delta)/a)$, for any ψ in $D(A)$, $\|A\Upsilon^u_{T,0}\psi\| \leq e^{\frac{2a}{\delta}TV_{[0,T]}(u)}\|A\psi\|$.

2.2 Definition of propagators for BV controls

For any $\delta \in (0,1)$ and $a > 0$, let $\mathcal{U}_{\delta,a}$ be the subset of $u \in \mathcal{U}$ such that $u : \mathbf{R} \to (-(1-\delta)/a, (1-\delta)/a)$.

Let u in $\mathcal{U}_{\delta,a}$. There exists a sequence u_n in $\mathcal{U}_{\delta,a}$ of piecewise constant functions such that (i) $(u_n)_n$ tends to u pointwise and (ii) for any n in $\mathbf{N}$, $TV_{[0,T]}(u_n) \leq TV_{[0,T]}(u)$. These conditions implies that $\sup_n \|u_n\|_{L^\infty} < +\infty$.

Proposition 4. Let (A,B) satisfy Hypothesis 1 with $b = 0$ and let $(u_n)_n$ be defined as above. For any t in $[0,T]$, for any ψ in $D(A)$, $(\Upsilon^{u_n}_{(t,0)}\psi)_{n\in\mathbf{N}}$ is a Cauchy sequence (for the norm of H).

Proof. By Duhamel's identity, for any ψ in $D(A)$,

$$
\Upsilon^{u_n}_{(t,0)}\psi - \Upsilon^{u_m}_{(t,0)}\psi = \int_0^t \Upsilon^{u_n}_{(s,t)}(u_n(s)-u_m(s))B\Upsilon^{u_m}_{(s,0)}\psi \mathrm{d}s
$$

For any s in $(0,t)$, by Proposition 3,

$$
\sup_{0\leq s\leq t\leq T}\sup_{n,m}\|\Upsilon^{u_n}_{(s,t)}B\Upsilon^{u_m}_{(s,0)}\psi\| < +\infty.
$$

Moreover, $u_n(s) - u_m(s)$ tends to zero as n,m tend to infinity ($(u_l(s))_l$ is a Cauchy sequence). The result follows from Lebesgue's dominated convergence theorem.

We define $\Upsilon^u_{(t,0)}\psi = \lim_n \Upsilon^{u_n}_{(t,0)}\psi$ for any ψ in $D(A)$. It is clear from the definition that the construction is independent on the choice the sequence $(u_n)_n$ converging to u. Since $D(A)$ is dense in H and $\Upsilon^u_{(t,0)}$ is bounded (in H norm) by 1 on $D(A)$, $\Upsilon^u_{(t,0)}$ admits an extension to H that we still denote with $\Upsilon^u_{(t,0)}$.

2.3 General case of A-bounded operators

Next proposition states that replacing A by $A_\lambda := A + \mathrm{i}\lambda\mathrm{Id}$ induces just a global phase shift at the level of the propagators.

Proposition 5. For any $\delta \in (0,1)$, any u in $\mathcal{U}_{\delta,a}$, for any (A,B) satisfying Hypothesis 1 with $b = 0$ in Hypothesis 1.4, for any λ in $\mathbf{R}$, denote with $\Upsilon^u_{t,0}$ and $\Upsilon^{u,\lambda}_{t,0}$ the propagators associated with $x' = (A+uB)x$ and $x' = (A_\lambda + uB)x$ respectively. Then $\Upsilon^{u,\lambda}_{t,0} = e^{\mathrm{i}\lambda t}\Upsilon^u_{t,0}$.

Proof. The result is obvious with piecewise constant controls. The result follows by taking the limit for a sequence of piecewise constant controls $(u_n)_n$ tending to u for the BV topology.

We now come back to the definition of propagators of (2) in the general case $\|B\psi\| \leq a\|A\psi\| + b\|\psi\|$. As A is bounded from below (Hypothesis 1.2), for every $\eta > 0$, there exists λ large enough such that $\|B\psi\| \leq (a+\eta)\|A_\lambda\psi\|$ and we apply the above procedure to (A_λ, B) to define the propagator $\Upsilon^{u,\lambda}_{t,0}$ and, finally, the propagator $\Upsilon^u_{t,0} := e^{-\mathrm{i}\lambda t}\Upsilon^{u,\lambda}_{t,0}$. Notice that this construction is independent on λ, provided that λ is large enough. Notice also, and this is instrumental in our study, that for any u with bounded variation such that $\sup|u| < 1/a$, for any λ large enough, $\|A\Upsilon^u_{t,0}\psi_0\| = \|A\Upsilon^{u,\lambda}_{t,0}\psi_0\|$ for every ψ_0 in $D(|A|)$.

Below we write $\Upsilon^{u,\lambda}_t$ for $\Upsilon^{u,\lambda}_{t,0}$ and $\|\psi\|_r$ for $\|(1+|A|)^r\psi\|$.

We sum up the result of Section 2 in the following Proposition.

Proposition 6. Let $\delta \in (0,1)$ and (A,B) satisfy Hypothesis 1. For any u in $\mathcal{U}_{\delta,a}$, for any $t \geq 0$, the propagator$\Upsilon^u_{t,0} : \psi \mapsto \Upsilon^u_{t,0}\psi$ is continuous from $D(|A|)$ to $D(|A|)$. Moreover, for every $\eta > 0$, there exists $\lambda \in \mathbf{R}$ such that, for any ψ in $D(A)$, for any u in $\mathcal{U}_{\delta,a}$, for any $t \geq 0$,

$$
\|(A+\mathrm{i}\lambda)\Upsilon^u_{t,0}\psi\| \leq e^{\frac{2a+\eta}{\delta}TV_{[0,t]}(u)}\|(A+\mathrm{i}\lambda)\psi\|.
$$

3. GOOD GALERKIN APPROXIMATIONS

For applications (design of control laws or numerical simulations), it is common to replace the original infinite dimensional system (2) by a suitable finite dimensional approximation. It is often possible to bound the error due to this approximation. Under Hypothesis 2, we derive in this section an explicit upper bound of this error that depends only on the L^1 norm and the total variation of the control. The results presented here extend the results of Boussaïd et al. (2012b).

3.1 Notion of Good Galerkin Approximations

Let $\mathbf{\Phi} = (\phi_j)_{j\in\mathbf{N}}$ be a Hilbert basis of H. For any N in $\mathbf{N}$, we define the orthogonal projection

$$
\pi^{\mathbf{\Phi}}_N\psi \in H \mapsto \sum_{j\leq N}\langle\phi_j,\psi\rangle\phi_j \in H.
$$

Definition 7. Let $(A,B,\Phi,1)$ satisfy Hypothesis 2 and $N \in \mathbf{N}$. The *Galerkin approximation* of (2) of order N is the system in H

$$
\dot{x} = (A^{(\mathbf{\Phi},N)} + u(t)B^{(\mathbf{\Phi},N)})x \qquad (7)
$$

where $A^{(\mathbf{\Phi},N)} = \pi^{\mathbf{\Phi}}_N A_{\restriction \mathrm{Im}\pi^{\mathbf{\Phi}}_N}$ and $B^{(\mathbf{\Phi},N)} = \pi^{\mathbf{\Phi}}_N B_{\restriction \mathrm{Im}\pi^{\mathbf{\Phi}}_N}$ are the *compressions* of A and B (respectively).

We denote by $X^u_{(\mathbf{\Phi},N)}(t,s)$ the propagator of (7) associated with a L^1 function u.

Remark 8. The operators $A^{(\mathbf{\Phi},N)}$ and $B^{(\mathbf{\Phi},N)}$ are defined on the *infinite* dimensional space H. However, they have finite rank and the dynamics of (Σ_N) leaves invariant the N-dimensional space $\mathcal{L}_N = \mathrm{span}_{1\leq j\leq N}\{\phi_j\}$. Thus, (Σ_N) can be seen as a finite dimensional bilinear system in $\mathcal{L}_N$.

The system (A,B) admits a sequence of *Good Galerkin Approximations* (GGA in short), in time $T \in (0,+\infty]$, for a functional norm $N(\cdot)$ on a functional space $\mathbf{U}$ in a subspace D (with norm $\|\cdot\|_D$) of H if, for any $K, \varepsilon > 0$, for any ψ in D, there exists N in $\mathbf{N}$ such that, for any u in $\mathbf{U}$, $N(u) \leq K$ implies $\|(X^u_{(\mathbf{\Phi},N)}(t,0) - \Upsilon^u_{t,0})\psi\|_D < \varepsilon$ for any $t < T$.

3.2 GGA for BV controls

Proposition 9. Let (A, B, Φ) satisfy Hypotheses 1, 2.2, 2.4 and 2.5. Then, for any $\delta \in (0,1)$, for any $r \in [0,1)$ for any $n \in \mathbf{N}$, $N \in \mathbf{N}$, $(\psi_j)_{1\leq j\leq n}$ in $D(|A|)^n$, and for any function u in $\mathcal{U}_{\delta,a}$,

$$\|(\mathrm{Id} - \pi_N^{\Phi})\Upsilon^u_t(\psi_j)\|_r \leq \frac{e^{\frac{2}{\delta}aTV_{\mathbf{R}}(u)}\|\psi_j\|_1}{\inf_{j>N}\lambda_j^{1-r}}. \quad (8)$$

for any $t \geq 0$ and $j = 1, \ldots, n$.

Proof. Fix $j \in \{1, \ldots, n\}$. For any $N > 1$, one has

$$\left\|(\mathrm{Id} - \pi_N^{\Phi})\Upsilon^u_{t,0}(\psi_j)\right\|_r^2 = \sum_{n=N+1}^{\infty} \lambda_n^{2r}|\langle\phi_n, \Upsilon^u_t(\psi_j)\rangle|^2$$
$$\leq \inf_{j>N} \lambda_j^{2(r-1)} \left\|\Upsilon^u_{t,0}(\psi_j)\right\|_1^2.$$

By Proposition 3, for any $t > 0$,

$$\|\Upsilon^u_{t,0}\psi_j\|_1 \leq e^{\frac{2}{\delta}aTV_{\mathbf{R}}(u)}\|\psi_j\|_1.$$

Proposition 10. (Good Galerkin Approximation). Let $\delta \in (0,1)$, $\alpha \in [0,1)$ and (A, B, Φ, α) satisfy Hypothesis 2. Then for any $\varepsilon > 0$, $K \geq 0$, $n \in \mathbf{N}$, and $(\psi_j)_{1\leq j\leq n}$ in $D(|A|)^n$ there exists $N \in \mathbf{N}$ such that for any L^1 function u in $\mathcal{U}_{\delta,a}$,

$\|u\|_{L^1} + TV_{\mathbf{R}}(u) < K \Rightarrow \|\Upsilon^u_t(\psi_j) - X^u_{(\mathbf{\Phi},N)}(t,0)\pi_N\psi_j\| < \varepsilon$, for any $t \geq 0$ and $j = 1, \ldots, n$.

Proof. Fix j in $\{1, \ldots, n\}$ and consider the map $t \mapsto \pi_N\Upsilon^u_t(\psi_j)$ that is absolutely continuous and satisfies, for almost any $t \geq 0$,

$$\frac{d}{dt}\pi_N\Upsilon^u_t(\psi_j) = (A^{(\mathbf{\Phi},N)} + u(t)B^{(\mathbf{\Phi},N)})\pi_N^{\Phi}\Upsilon^u_t(\psi_j)$$
$$+ u(t)\pi_N^{\Phi}B(\mathrm{Id} - \pi_N^{\Phi})\Upsilon^u_t(\psi_j).$$

Hence, by variation of constants, for any $t \geq 0$,

$$\pi_N\Upsilon^u_t(\psi_j) = X^u_{(\mathbf{\Phi},N)}(t,0)\pi_N^{\Phi}\psi_j$$
$$+ \int_0^t X^u_{(\mathbf{\Phi},N)}(t,s)\pi_N^{\Phi}B(\mathrm{Id} - \pi_N)\Upsilon^u_s(\psi_j)u(\tau)\mathrm{d}\tau. \quad (9)$$

By Proposition 9, the norm of $t \mapsto B(\mathrm{Id} - \pi_N)\Upsilon^u_t(\psi_j)$ is less than $de^{\frac{2}{\delta}aK}\inf_{j>N}\lambda_j^{\alpha-1}\|\psi_j\|_1$. Since $X^u_{(\mathbf{\Phi},N)}(t,s)$ is unitary,

$$\|\pi_N\Upsilon^u_t(\psi_j) - X^u_{(\mathbf{\Phi},N)}(t,0)\pi_N\psi_j\|$$
$$\leq \|u\|_{L^1} d \inf_{j>N} \lambda_j^{\alpha-1} e^{c(A,B)K}\|\psi_j\|_1.$$

Then

$$\|\Upsilon^u_t(\psi_j) - X^u_{(N)}(t,0)\pi_N^{\Phi}\psi_j\|$$
$$\leq \|(\mathrm{Id} - \pi_N)\Upsilon^u_t(\psi_j)\| + \|\pi_N^{\Phi}\Upsilon^u_t(\psi_j) - X^u_{(\mathbf{\Phi},N)}(t,0)\pi_N^{\Phi}\psi_j\|$$
$$\leq \|u\|_{L^1}(1 + dK)de^{\frac{2}{\delta}aK} \inf_{j>N} \lambda_j^{\alpha-1}\|\psi_j\|_1.$$

This completes the proof since λ_n tends to infinity as n goes to infinity.

4. EXAMPLES

4.1 Tri-diagonal systems

Definition 11. A system $(A, B, \mathbf{\Phi})$ is *tri-diagonal* if (A, B) satisfies Hypotheses 1.1, 1.2, 1.3, 2.2, 2.4 and 2.5 and if, for any j, k in $\mathbf{N}$, $|j - k| > 1$ implies $\langle\phi_j, B\phi_k\rangle = 0$.

In the following, we denote $b_{j,k} = \langle\phi_j, B\phi_k\rangle$.

Proposition 12. Let $(A, B, \mathbf{\Phi})$ be a tri-diagonal system and let r be a positive number. Assume that the sequences $\left(\frac{b_{n,n-1}}{\lambda_n^r}\right)_{n\in\mathbf{N}}$, $\left(\frac{b_{n,n}}{\lambda_n^r}\right)_{n\in\mathbf{N}}$ and $\left(\frac{b_{n,n+1}}{\lambda_n^r}\right)_{n\in\mathbf{N}}$ are bounded by C. Then, for any ψ in $D(|A|^r)$, $\|B\psi\| \leq \sqrt{6}C\||A|^r\psi\|$. In particular, if $r \leq 1$ (resp. $r < 1$), then (A, B) satisfies Hypothesis 1 (resp. $(A, B, \mathbf{\Phi}, r)$ satisfies Hypothesis 2).

Proof. For any ψ in $D(|A|^r)$,

$$\|B\psi\|^2 = \left\|\sum_{k\in\mathbf{N}}\langle\phi_k, B\psi\rangle\phi_k\right\|^2 = \sum_{k\in\mathbf{N}}|\langle B\phi_k, \psi\rangle|^2$$
$$= \sum_{k\in\mathbf{N}}|b_{k-1,k}\langle\phi_{k-1}, \psi\rangle + b_{k,k}\langle\phi_k, \psi\rangle + b_{k+1,k}\langle\phi_{k+1}, \psi\rangle|^2$$
$$\leq 2\sum_{k\in\mathbf{N}}|b_{k,k-1}|^2|\langle\phi_{k-1}, \psi\rangle|^2 + |b_{k,k}|^2|\langle\phi_k, \psi\rangle|^2$$
$$+ |b_{k,k+1}|^2|\langle\phi_{k+1}, \psi\rangle|^2$$
$$\leq 2C^2\sum_{k\in\mathbf{N}}(\lambda_{k-1}^{2r}|\langle\phi_{k-1}, \psi\rangle|^2 + \lambda_k^{2r}|\langle\phi_k, \psi\rangle|^2$$
$$+ \lambda_{k+1}^{2r}|\langle\phi_{k+1}, \psi\rangle|^2)$$
$$\leq 6C^2\||A|^r\psi\|^2 \quad (10)$$

4.2 A toy model: the anharmonic oscillator

Consider the system

$$\mathrm{i}\frac{\partial\psi}{\partial t}(x,t) = [(-\Delta + x^2)^{\alpha} + u(t)x^{\beta}]\psi(x,t), \quad (11)$$

with x in $\mathbf{R}$, ψ in $L^2(\mathbf{R}, \mathbf{C})$, α, β in $\mathbf{N}$. When $\alpha = \beta = 1$, (11) is one of the most important quantum system, it is the standard quantum harmonic oscillator submitted to a uniform electric field. For $\beta = 1$ the system is tri-diagonal.

With our notations, $H = L^2(\mathbf{R}, \mathbf{C})$, $A : \psi \mapsto -\mathrm{i}(-\Delta + x^2)^{\alpha}\psi$ and $B : \psi \mapsto -\mathrm{i}x^{\beta}\psi$. Operator A is skew-adjoint on its domain $D(A)$, B is skew-symmetric. A Hilbert basis $\mathbf{\Phi}$ of $L^2(\mathbf{R}, \mathbf{C})$ made of eigenvectors of A is given by the sequence $(\phi_k)_{k\in\mathbf{N}}$ of the normalized Hermite functions

$$\phi_k : x \mapsto (-1)^k(2^k k!\sqrt{\pi})^{-1/2}e^{x^2/2}\frac{\mathrm{d}^k}{\mathrm{d}x^k}e^{-x^2}.$$

For any k in $\mathbf{N}$, the eigenvector ϕ_k is associated with the eigenvalue $-\mathrm{i}\lambda_k = -\mathrm{i}(2k+1)^{\alpha}$.

Proposition 13. If $2\alpha \geq \beta$ then system (11) satifies Hypothesis 1. If $2\alpha > \beta$ then system (11) satifies Hypothesis 2.

Proof. We show that the system satisfies Hypothesis 1.4 if $2\alpha \geq \beta$ and Hypothesis 2.6 if $2\alpha > \beta$. The system clearly fulfills all other hypotheses. For any k in $\mathbf{N}$,

$$x\phi_k(x) = \sqrt{\frac{k}{2}}\phi_{k-1}(x) + \sqrt{\frac{k+1}{2}}\phi_{k+1}(x).$$

Iterating β times this equality, one gets for any k,

$$|\langle x^\beta \phi_k, \psi\rangle| \leq ((k+\beta)/2)^{\beta/2} \sum_{j=-\beta}^{\beta} |\langle \phi_{k+j}, \psi\rangle|$$

hence, following the idea of the chain of inequalities (10) one has

$$\begin{aligned}\|B\psi\|^2 &= \sum_{k\in\mathbf{N}} |\langle B\phi_k, \psi\rangle|^2 \\ &\leq C\|\psi\|^2 + 2^{-\beta} \sum_{k>\beta} (k+\beta)^\beta \sum_{j=-\beta}^{\beta} |\langle \phi_{k+j}, \psi\rangle|^2 \\ &\leq C\|\psi\|^2 + 2^{-\beta} \sum_{j=-\beta}^{\beta} \sum_{k>\beta} (2k+1)^\beta |\langle \phi_{k+j}, \psi\rangle|^2 \\ &\leq C\|\psi\|^2 + 2^{-\beta}(2\beta+1)\||A|^{\beta/(2\alpha)}\psi\|^2,\end{aligned}$$

which concludes the proof.

Thanks to Proposition 13, we can apply Proposition 6 and prove the well-posedness of (11)

Proposition 14. If $2\alpha = \beta$, then (11) is well-posed for any control u with bounded variation and L^∞ norm smaller than $\sqrt{(2\beta+1)2^{-\beta}}$. If $2\alpha > \beta$, then (11) is well-posed for any control u of bounded variation.

Notice that Proposition 10 applies also to systems that are *not* weakly-coupled, see (Boussaïd et al., 2013, Definition 1). For instance, using the set $\{(k, k+1), k \in \mathbf{N}\}$ as a non-resonant chain of connectedness, see (Boscain et al., 2012, Definition 2.5), and the fact that $(|b_{k,k+1}|^{-1})_{k\in\mathbf{N}}$ is in ℓ^1, we get the following.

Proposition 15. Assume that $\beta \geq 3$ odd and $\alpha > \beta/2$. Then, there exists $K = \sum_k \frac{2\pi}{|b_{k,k+1}|} > 0$ such that, for any even functions ψ_0, ψ_1 in the unit sphere of $L^2(\mathbf{R}, \mathbf{C})$, for any $\varepsilon > 0$, there exists a control $u_\varepsilon : [0, T_\varepsilon] \to [0, +\infty)$ such that $\|\Upsilon^{u_\varepsilon}_{T_\varepsilon,0}\psi_0 - \psi_1\|_{L^2} \leq \varepsilon$ and $\|u_\varepsilon\|_{L^1([0,T_\varepsilon])} < K$.

In other words, if $2\alpha > \beta \geq 3$ and β is odd, then there is no Good Galerkin approximation for (11) in $L^2(\mathbf{R}, \mathbf{C})$ in terms of the L^1 norm of the control. However, from Proposition 10, system (11) admits a sequence of Good Galerkin approximations in $L^2(\mathbf{R}, \mathbf{C})$ in terms of the $(L^1 + TV)$ norm of the control.

4.3 Rotation of a 2D molecule

We consider a linear molecule whose only degree of freedom is the planar rotation, in a fixed plan, about its fixed center of mass. In this model, the Schrödinger equation reads

$$\mathrm{i}\frac{\partial \psi}{\partial t} = -\Delta\psi + \cos\theta\psi, \quad \theta \in \Omega, \tag{12}$$

$\Omega = \mathbf{R}/2\pi\mathbf{Z}$ is the unit circle endowed with the Riemannian structure inherited from $\mathbf{R}$, H is the space of odd functions of $L^2(\Omega, \mathbf{C})$, $A = \mathrm{i}\Delta$ (Δ is the restriction to H of the Laplace-Beltrami operator of Ω) and $B : \psi \mapsto (\theta \mapsto \cos(\theta)\psi(\theta))$ is the multiplication by cosine.

In the Hilbert basis $\Phi = (\theta \mapsto \sin(k\theta))_{k\in\mathbf{N}}$ of H, A is diagonal with diagonal $-\mathrm{i}k^2, k = 1\ldots\infty$ and B is tri-diagonal with $b_{k,k} = 0, b_{k,k+1} = -\mathrm{i}/2$ for every k in $\mathbf{N}$.

System 12 is both tri-diagonal and weakly-coupled and it has been thoroughly studied (see for instance Boscain et al. (2009) and Boscain et al. (2012)). For instance, it was known that (12) admits a sequence of Good Galerkin Approximations in terms of L^1 norm of the control. More preciselyby (Boussaïd et al., 2013, Section IV.C)) for every ϕ with norm 1 in span(ϕ_1, ϕ_2),

$$\|X^u_{(\Phi,N)}(t,0)\phi - \pi^\Phi_N \Upsilon^u_t(\phi)\| \leq \frac{K^{N-1}}{(N-2)!}.$$

Approximate controllability of (12) was established in Boscain et al. (2012). In Chambrion (2012) is given an explicit control law to steer (12) from ϕ_1 to any neighborhood of ϕ_2 using periodic functions with frequency $2\pi/3$. Defining $u_n := t \mapsto \cos(3t)/n$ and $T^* = 2\pi$, we have $\left|\langle \phi_2, \Upsilon^{u_n}_{nT^*,0}\phi_1\rangle\right| \leq \dfrac{9}{n}$. Since $\|B\psi\| \leq \sqrt{2}\|A\psi\|$ for every ψ in $D(A)$, Proposition 3 implies that every control $u : [0,T] \to \{0,1\}$ with bounded variation satisfying $|\langle \phi_2, \Upsilon^u_{T,0}\phi_1\rangle| > 1 - \varepsilon$ has total variation larger than $\log(2(1-\varepsilon))/4$. This lower bound is rather conservative, and we will give better estimates using the boundedness of B.

For every u_1, u_2, t_1, t_2 in $\mathbf{R}$, for every ψ in H, one has

$$\begin{aligned}&\|(A + u_1B)e^{t(A+u_2B)}\psi\| \\ &= \|(A + u_2B)e^{t(A+u_2B)}\psi + (u_2 - u_1)Be^{t(A+u_2B)}\psi\| \\ &\leq \|(A + u_2B)e^{t(A+u_2B)}\psi\| + \|(u_2 - u_1)Be^{t(A+u_2B)}\psi\| \\ &\leq \|(A + u_2B)\psi\| + |u_2 - u_1|\|B\|\|\psi\|\end{aligned}$$

For every $u_1, u_2, \ldots, u_n$ and $t_1, t_2, \ldots, t_n$ in $\mathbf{R}$, for every ψ in the unit sphere of H, one shows by induction on n that

$$\begin{aligned}&\|Ae^{t_1(A+u_1B)}e^{t_2(A+u_2B)}\cdots e^{t_n(A+u_nB)}\psi\| \\ &\leq \|A\psi\| + \|B\|(|u_1| + |u_2 - u_1| + \cdots + |u_n - u_{n-1}| + |u_n|)\end{aligned}$$

Let k in $\mathbf{N}$ and ψ in an ε-neighborhood of ϕ_k. If u is piecewise constant taking value in $\{0,1\}$, with $u(0) = 0 = \lim_{t\to\infty} u(t)$, such that $\Upsilon^u_t\phi_1 = \psi$, then the number $\mathcal{N}$ of switches of u satisfies $\|A\psi\| \leq \|A\phi_1\| + \|B\|\mathcal{N}$, or

$$\mathcal{N} \geq \frac{\|A\phi_k\| - k^2\varepsilon - \|A\phi_1\|}{\|B\|} = \frac{k^2(1-\varepsilon) - 1}{\sqrt{2}}.$$

4.4 Cooling in harmonic traps

This example is inspired by H. R. Lewis and Riesenfeld (1969). The dynamics of a quantum system trapped in a one-dimensional parabolic potential with time varying frequency $\omega(t)$ is given by

$$\mathrm{i}\frac{\partial \psi}{\partial t}(x,t) = (-\Delta + \omega(t)x^2)\psi(x,t), \tag{13}$$

The system (13) has raised considerable attention in the last decades (see Stefanatos et al. (2011) for recent developments).

Let $\lambda > 0$. Defining $u(t) := \omega(t) - \lambda$, we reformulate (13) as

$$\mathrm{i}\frac{\partial \psi}{\partial t}(x,t) = (-\Delta + \lambda x^2 + u(t)x^2)\psi(x,t), \tag{14}$$

Note that the parity, if any, of the solutions of (13) is preserved along the time. Hence we consider (14) in the space H of even functions in $L^2(\mathbf{R}, \mathbf{C})$. For any $\lambda > 0$, in the basis $\Phi = (x \mapsto \frac{1}{\lambda^{1/4}} H_{2k}(\sqrt{\lambda}x))_{k\in\mathbf{N}}$, where H_n is the

n^{th} Hermite functions, the operator $A_\lambda := \mathrm{i}(-\Delta+\lambda^2 x^2)_{|H}$ is diagonal with diagonal $((2k+1)\lambda)_{k\in\mathbf{N}}$ and $B = -\mathrm{i}x^2_{|H}$ has matrix $[b_{j,k}]_{(j,k)\in\mathbf{N}^2}$ with $b_{j,k}=0$ if $|j-k|>1$ and $b_{j,j}\sim_\infty j/\lambda$ and $b_{j,j+1}\sim_\infty j/(2\lambda)$ for any j,k in $\mathbf{N}^2$.

The system (A_λ, B) is tri-diagonal and the well-posedness of (13) follows as in Propositions 12 and 6 applied to (14) with u any control with bounded variation and small enough.

Proposition 16. For any even function ψ_0 in $L^2(\mathbf{R},\mathbf{C})$, for any $T>0$, for any $\alpha>0$, for any $\omega:[0,T]\to(\alpha,+\infty)$ with bounded variation, (13) admits a unique solution $t\mapsto \Upsilon^\omega_t\psi_0$ satisfying $\Upsilon^\omega_0\psi_0=\psi_0$.

5. CONCLUSION

We obtained an elementary proof of the well-posedness of bilinear Schrödinger equations by adapting classical tools developed by Kato to the simple structure of bilinear conservative systems. The key ingredient of our construction is an *a priori* upper bound on the growth of some energy functional in terms of the total variation of the control.

As a consequence we prove a general method to obtain explicit bounds on the number of switches of a control steering the system from a given source to a given target, in the case in which the control takes value in a discrete set. These bounds are of importance when considering quantum systems for which the dipolar approximation (leading to a bilinear modeling as in the present paper) is not valid anymore, see Morancey (2011) and Boussaïd et al. (2012a).

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